

## Author Index to Volume 181

- Abramczyk, H., M. Barut, A. Ben Altabef and R. Escibano, Vibrational dephasing of axial and equatorial conformers in cyclohexyl bromide 181 (1994) 393
- Abramczyk, H., see A. Ben Altabef 181 (1994) 401
- Ågren, H., see B.F. Minaev 181 (1994) 15
- Ågren, H., O. Vahtras, S. Knuts and P. Jørgensen, Radiative lifetimes of triplet spin sublevels of the azabenzenes 181 (1994) 291
- Asselin, P., F. Piuze, J. Le Calvé, M. Mons and I. Dimicoli, Rydberg states of gas phase chlorobenzene observed by double resonance multiphoton ionization photoelectron spectroscopy 181 (1994) 271
- Baklanov, A.V. and A.I. Chichinin, Time-resolved LMR measurement of the rate constants of the reactions  $\text{SiH}_3 + \text{SiH}_3$  and  $\text{SiH}_3 + \text{Cl}$  181 (1994) 119
- Bancroft, G.M., see J.N. Cutler 181 (1994) 461
- Barut, M., see H. Abramczyk 181 (1994) 393
- Barzoukas, M., see M. Blanchard-Desce 181 (1994) 281
- Bäuerle, P., see P. Emele 181 (1994) 417
- Bazalgette, G., see A. Durand 181 (1994) 209
- Ben Altabef, A., see H. Abramczyk 181 (1994) 393
- Ben Altabef, A., R. Escibano and H. Abramczyk, Vibrational dephasing of axial and equatorial conformers in cyclohexyl chloride and in 4-chloro-oxacyclohexane 181 (1994) 401
- Blanchard-Desce, M., J.-M. Lehn, M. Barzoukas, I. Ledoux and J. Zyss, Chain-length dependence of the quadratic hyperpolarizability of push-pull polyenes and carotenoids. Effect of end groups and conjugation path 181 (1994) 281
- Bluhm, H., J. Lindner and E. Tiemann, Double resonance spectroscopy of NaI and KI: the van der Waals states  $\Omega=1$  and  $\Omega=2$  of the first atomic asymptote 181 (1994) 173
- Bo, C., J.M. Maestre, J.M. Poblet and J.M. Ricart, Chemisorption of aluminium and chlorine on the Si(111) surface. An ab initio study of the nature of the interaction 181 (1994) 63
- Borshch, S.A. and J.-J. Girerd, Vibronic reduction of electron transfer in strongly correlated molecular models 181 (1994) 1
- Brańka, A.C. and K.W. Wojciechowski, Equation of state of planar hard molecular fluids; hard cyclic multimer system 181 (1994) 29
- Brion, C.E., see G.R. Burton 181 (1994) 147
- Brosolo, M., P. Decleva and A. Lisini, LCAO expansion in a spline basis for accurate variational determination of continuum wavefunctions. Applications to  $\text{H}_2^+$  and  $\text{HeH}^{2+}$  181 (1994) 85
- Bultmann, T., see A. Mühlfordt 181 (1994) 447
- Burton, G.R., W.F. Chan, G. Cooper and C.E. Brion, Valence- and inner-shell (Cl 2p, 2s; C 1s) photoabsorption and photoionization of carbon tetrachloride. Absolute oscillator strengths (5–400 eV) and dipole-induced breakdown pathways 181 (1994) 147
- Cavagnat, R., see C. Sourisseau 181 (1994) 377

## Author Index to Volume 181

- Abramczyk, H., M. Barut, A. Ben Altabef and R. Escibano, Vibrational dephasing of axial and equatorial conformers in cyclohexyl bromide 181 (1994) 393
- Abramczyk, H., see A. Ben Altabef 181 (1994) 401
- Ågren, H., see B.F. Minaev 181 (1994) 15
- Ågren, H., O. Vahtras, S. Knuts and P. Jørgensen, Radiative lifetimes of triplet spin sublevels of the azabenzenes 181 (1994) 291
- Asselin, P., F. Piuze, J. Le Calvé, M. Mons and I. Dimicoli, Rydberg states of gas phase chlorobenzene observed by double resonance multiphoton ionization photoelectron spectroscopy 181 (1994) 271
- Baklanov, A.V. and A.I. Chichinin, Time-resolved LMR measurement of the rate constants of the reactions  $\text{SiH}_3 + \text{SiH}_3$  and  $\text{SiH}_3 + \text{Cl}$  181 (1994) 119
- Bancroft, G.M., see J.N. Cutler 181 (1994) 461
- Barut, M., see H. Abramczyk 181 (1994) 393
- Barzoukas, M., see M. Blanchard-Desce 181 (1994) 281
- Bäuerle, P., see P. Emele 181 (1994) 417
- Bazalgette, G., see A. Durand 181 (1994) 209
- Ben Altabef, A., see H. Abramczyk 181 (1994) 393
- Ben Altabef, A., R. Escibano and H. Abramczyk, Vibrational dephasing of axial and equatorial conformers in cyclohexyl chloride and in 4-chloro-oxacyclohexane 181 (1994) 401
- Blanchard-Desce, M., J.-M. Lehn, M. Barzoukas, I. Ledoux and J. Zyss, Chain-length dependence of the quadratic hyperpolarizability of push-pull polyenes and carotenoids. Effect of end groups and conjugation path 181 (1994) 281
- Bluhm, H., J. Lindner and E. Tiemann, Double resonance spectroscopy of NaI and KI: the van der Waals states  $\Omega=1$  and  $\Omega=2$  of the first atomic asymptote 181 (1994) 173
- Bo, C., J.M. Maestre, J.M. Poblet and J.M. Ricart, Chemisorption of aluminium and chlorine on the Si(111) surface. An ab initio study of the nature of the interaction 181 (1994) 63
- Borshch, S.A. and J.-J. Girerd, Vibronic reduction of electron transfer in strongly correlated molecular models 181 (1994) 1
- Brańka, A.C. and K.W. Wojciechowski, Equation of state of planar hard molecular fluids; hard cyclic multimer system 181 (1994) 29
- Brion, C.E., see G.R. Burton 181 (1994) 147
- Brosolo, M., P. Decleva and A. Lisini, LCAO expansion in a spline basis for accurate variational determination of continuum wavefunctions. Applications to  $\text{H}_2^+$  and  $\text{HeH}^{2+}$  181 (1994) 85
- Bultmann, T., see A. Mühlfordt 181 (1994) 447
- Burton, G.R., W.F. Chan, G. Cooper and C.E. Brion, Valence- and inner-shell (Cl 2p, 2s; C 1s) photoabsorption and photoionization of carbon tetrachloride. Absolute oscillator strengths (5–400 eV) and dipole-induced breakdown pathways 181 (1994) 147
- Cavagnat, R., see C. Sourisseau 181 (1994) 377

- Chan, W.F., see G.R. Burton 181 (1994) 147
- Chandra, A.K., see R. Sumathi 181 (1994) 73
- Chichinin, A.I., see A.V. Baklanov 181 (1994) 119
- Chow, Y.L., see T.O. Harju 181 (1994) 259
- Cooper, G., see G.R. Burton 181 (1994) 147
- Cukrowski, A.S., S. Fritzsche and W. Stiller, Synergistic effects in bimolecular reactions in a dilute gas 181 (1994) 7
- Cutler, J.N., G.M. Bancroft and K.H. Tan, High-resolution Ge 3d and Sn 4d core-level photoelectron spectra. Ligand field and vibrational effects 181 (1994) 461
- Dalby, F.W., see A. Durand 181 (1994) 209
- Decleva, P., see M. Brosolo 181 (1994) 85
- Dick, B., see A. Mühlfordt 181 (1994) 447
- Dimicoli, I., see P. Asselin 181 (1994) 271
- Durand, A., J.C. Loison, G. Bazalgette, E. Gangler, F.W. Dalby and J. Vigué, On the B state of the ICl molecule: hyperfine structure and hyperfine predissociation 181 (1994) 209
- Dyke, J.M., D. Haggerston, M.P. Hastings and T.G. Wright, A He(I) photoelectron spectroscopic study of MgF<sub>2</sub> in the gas phase 181 (1994) 355
- Effenberger, F., see P. Emele 181 (1994) 417
- Eikema, K.S.E., W. Hogervorst and W. Ubachs, Predissociation rates in carbon monoxide: dependence on rotational state, parity and isotope 181 (1994) 217
- Emele, P., D.U. Meyer, N. Holl, H. Port, H.C. Wolf, F. Würthner, P. Bäuerle and F. Effenberger, Dual fluorescence of 9-anthryl-substituted oligothiophenes in nonpolar environment 181 (1994) 417
- Ernsting, N.P., see A. Mühlfordt 181 (1994) 447
- Erostyák, J., see T.O. Harju 181 (1994) 259
- Escribano, R., see H. Abramczyk 181 (1994) 393
- Escribano, R., see A. Ben Altabef 181 (1994) 401
- Eviatar, H., E.E. van Faassen, Y.K. Levine and D.I. Hoult, Time-domain simulation of ESR spectra of nitroxide spin probes 181 (1994) 369
- Ferrari, L., A new drift-velocity formula for ions in lighter gases in an electric field 181 (1994) 319
- Ferretti, A. and A. Lami, Optical properties of linear mixed valence coordination compounds by two-band Hubbard Hamiltonian 181 (1994) 107
- Fisz, J.J., Fluorescence depolarization of solutions and ordered systems. Photochemical reactions in the excited states. II. General considerations (b) 181 (1994) 425
- Fouassier, M., see C. Sourisseau 181 (1994) 377
- Fritzsche, S., see A.S. Cukrowski 181 (1994) 7
- Galasso, V., Theoretical study of the nuclear spin-spin coupling constant of the ultrashort central bond in bitetrahedrane 181 (1994) 363
- Gangler, E., see A. Durand 181 (1994) 209
- Girerd, J.-J., see S.A. Borshch 181 (1994) 1
- Gorecki, J. and I. Hanazaki, A simple phenomenological model for nonequilibrium interaction between two reactions in a Lorentz gas 181 (1994) 39

- Ha, T.-K. and C. Puebla, A theoretical study of conformations and vibrational frequencies in  $(\text{NH}_2)_2\text{C}=\text{X}$  compounds ( $\text{X}=\text{O}$ ,  $\text{S}$ , and  $\text{Se}$ ) 181 (1994) 47
- Haggerston, D., see J.M. Dyke 181 (1994) 355
- Hanazaki, I., see J. Gorecki 181 (1994) 39
- Harju, T.O., J. Erostryák, Y.L. Chow and J.E.I. Korppi-Tommola, The isomerization reaction of electronically excited (dibenzylmethine)borondifluoride in *n*-alcohols. Study of microscopic friction and polarity 181 (1994) 259
- Hastings, M.P., see J.M. Dyke 181 (1994) 355
- Hogervorst, W., see K.S.E. Eikema 181 (1994) 217
- Hohlneicher, G., see J. Wolf 181 (1994) 185
- Holl, N., see P. Emele 181 (1994) 417
- Hoult, D.I., see H. Eviatar 181 (1994) 369
- Hubinger, S. and J.B. Nee, Photoabsorption spectrum for OCIO between 125 and 470 nm 181 (1994) 247
- Ichikawa, H., see H. Tokiwa 181 (1994) 97
- Jørgensen, P., see H. Ågren 181 (1994) 291
- Kikuchi, O., see H. Takase 181 (1994) 57
- Knuts, S., see B.F. Minaev 181 (1994) 15
- Knuts, S., see H. Ågren 181 (1994) 291
- Korppi-Tommola, J.E.I., see T.O. Harju 181 (1994) 259
- Lami, A., see A. Ferretti 181 (1994) 107
- Le Calvé, J., see P. Asselin 181 (1994) 271
- Ledoux, I., see M. Blanchard-Desce 181 (1994) 281
- Lehn, J.-M., see M. Blanchard-Desce 181 (1994) 281
- Levant, R., see C. Lugez 181 (1994) 129
- Levine, Y.K., see H. Eviatar 181 (1994) 369
- Lindner, J., see H. Bluhm 181 (1994) 173
- Lisini, A., see M. Brosolo 181 (1994) 85
- Loison, J.C., see A. Durand 181 (1994) 209
- Lugez, C., A. Schriver, R. Levant and L. Schriver-Mazzuoli, A matrix-isolation infrared spectroscopic study of the reactions of methane and methanol with ozone 181 (1994) 129
- Maestre, J.M., see C. Bo 181 (1994) 63
- Meyer, D.U., see P. Emele 181 (1994) 417
- Miljanić, Š.S., see M.S. Trtica 181 (1994) 409
- Minaev, B.F., S. Knuts and H. Ågren, On the interpretation of the external heavy atom effect on singlet-triplet transitions 181 (1994) 15
- Mons, M., see P. Asselin 181 (1994) 271
- Morales, J., see C. Sourisseau 181 (1994) 377
- Mühlpfordt, A., T. Bultmann, N.P. Ernsting and B. Dick, Excited-state intramolecular proton transfer in jet-cooled 3-hydroxyflavone. Deuteration studies, vibronic double-resonance experiments, and semiempirical (AM1) calculations of potential-energy surfaces 181 (1994) 447
- Nee, J.B., see S. Hubinger 181 (1994) 247

- Osamura, Y., see H. Tokiwa 181 (1994) 97
- Piuzzi, F., see P. Asselin 181 (1994) 271
- Poblet, J.M., see C. Bo 181 (1994) 63
- Port, H., see P. Emele 181 (1994) 417
- Puebla, C., see T.-K. Ha 181 (1994) 47
- Ricart, J.M., see C. Bo 181 (1994) 63
- Savel'ev, V.A., see N.D. Sokolov 181 (1994) 305
- Schrivier, A., see C. Lugez 181 (1994) 129
- Schrivier-Mazzuoli, L., see C. Lugez 181 (1994) 129
- Sokolov, N.D. and V.A. Savel'ev, Isotope effects in weak hydrogen bonds. Allowance for two stretching and two bending modes of the A-H...B fragment 181 (1994) 305
- Sourisseau, C., R. Cavagnat, M. Fouassier, J.L. Tirado and J. Morales, Optical, Raman and resonance Raman spectra and lattice dynamics calculations of the misfit layer compounds, (SnS)<sub>1.17</sub>NbS<sub>2</sub> and (PbS)<sub>1.18</sub>TiS<sub>2</sub> 181 (1994) 377
- Stillier, W., see A.S. Cukrowski 181 (1994) 7
- Sumathi, R. and A.K. Chandra, Dissociation dynamics of acetyl chloride and cis-trans isomerisation of methoxychloro carbene and chlorohydroxymethyl carbene 181 (1994) 73
- Takase, H. and O. Kikuchi, Monte Carlo and molecular orbital study of the (CH<sub>3</sub>)<sub>2</sub>NO radical in solution 181 (1994) 57
- Tan, K.H., see J.N. Cutler 181 (1994) 461
- Tiemann, E., see H. Bluhm 181 (1994) 173
- Tirado, J.L., see C. Sourisseau 181 (1994) 377
- Tokiwa, H., Y. Osamura and H. Ichikawa, Energy-component analysis along zero virial path 181 (1994) 97
- Trtica, M.S. and Š.S. Miljanić, Investigation of gas chemistry in the sealed TEA CO<sub>2</sub> laser 181 (1994) 409
- Ubachs, W., see K.S.E. Eikema 181 (1994) 217
- Vahtras, O., see H. Ågren 181 (1994) 291
- Van Faassen, E.E., see H. Eviatar 181 (1994) 369
- Vigué, J., see A. Durand 181 (1994) 209
- Wilson, L.C., Development of non-local Wigner-like correlation-energy density functionals through coordinate scaling requirements and evaluation of constraint obedience in the construction of density functionals 181 (1994) 337
- Wojciechowski, K.W., see A.C. Brańka 181 (1994) 29
- Wolf, H.C., see P. Emele 181 (1994) 417
- Wolf, J. and G. Hohlneicher, High-resolution one- and two-photon spectra of matrix-isolated anthracene 181 (1994) 185
- Wright, T.G., see J.M. Dyke 181 (1994) 355
- Würthner, F., see P. Emele 181 (1994) 417
- Zyss, J., see M. Blanchard-Desce 181 (1994) 281

## Subject Index to Volume 181

### Methods

#### Theoretical

##### *Many body and quasiparticle approaches*

- Vibronic reduction of electron transfer in strongly correlated molecular models, S.A. Borshch and J.-J. Girerd 181 (1994) 1

##### *Coupling schemes and perturbative treatments*

- Vibronic reduction of electron transfer in strongly correlated molecular models, S.A. Borshch and J.-J. Girerd 181 (1994) 1
- Synergistic effects in bimolecular reactions in a dilute gas, A.S. Cukrowski, S. Fritzsche and W. Stiller 181 (1994) 7
- On the interpretation of the external heavy atom effect on singlet-triplet transitions, B.F. Minaev, S. Knuts and H. Ågren 181 (1994) 15
- Radiative lifetimes of triplet spin sublevels of the azabenzenes, H. Ågren, O. Vahtras, S. Knuts and P. Jørgensen 181 (1994) 291
- Isotope effects in weak hydrogen bonds. Allowance for two stretching and two bending modes of the A-H...B fragment, N.D. Sokolov and V.A. Savel'ev 181 (1994) 305

##### *Equilibrium statistical mechanics*

- Equation of state of planar hard molecular fluids; hard cyclic multimer system, A.C. Brańka and K.W. Wojciechowski 181 (1994) 29

##### *Statistical mechanics of stationary states*

- A new drift-velocity formula for ions in lighter gases in an electric field, L. Ferrari 181 (1994) 319

##### *Non-equilibrium thermodynamic and hydrodynamic theories*

- A simple phenomenological model for nonequilibrium interaction between two reactions in a Lorentz gas, J. Gorecki and I. Hanazaki 181 (1994) 39

##### *Ab initio schemes for stationary properties*

- A theoretical study of conformations and vibrational frequencies in  $(\text{NH}_2)_2\text{C}=\text{X}$  compounds ( $\text{X}=\text{O}, \text{S}, \text{and Se}$ ), T.-K. Ha and C. Puebla 181 (1994) 47
- Monte Carlo and molecular orbital study of the  $(\text{CH}_3)_2\text{NO}$  radical in solution, H. Takase and O. Kikuchi 181 (1994) 57
- Chemisorption of aluminium and chlorine on the Si(111) surface. An ab initio study of the nature of the interaction, C. Bo, J.M. Maestre, J.M. Poblet and J.M. Ricart 181 (1994) 63
- Dissociation dynamics of acetyl chloride and cis-trans isomerisation of methoxychloro carbene and chlorohydroxymethyl carbene, R. Sumathi and A.K. Chandra 181 (1994) 73

- LCAO expansion in a spline basis for accurate variational determination of continuum wavefunctions. Applications to  $\text{H}_2^+$  and  $\text{HeH}^{2+}$ , M. Brosolo, P. Decleva and A. Lisini 181 (1994) 85
- Energy-component analysis along zero virial path, H. Tokiwa, Y. Osamura and H. Ichikawa 181 (1994) 97
- Radiative lifetimes of triplet spin sublevels of the azabenzenes, H. Ågren, O. Vahtras, S. Knuts and P. Jørgensen 181 (1994) 291
- Development of non-local Wigner-like correlation-energy density functionals through coordinate scaling requirements and evaluation of constraint obedience in the construction of density functionals, L.C. Wilson 181 (1994) 337
- A He(I) photoelectron spectroscopic study of  $\text{MgF}_2$  in the gas phase, J.M. Dyke, D. Haggerston, M.P. Hastings and T.G. Wright 181 (1994) 355
- Theoretical study of the nuclear spin-spin coupling constant of the ultrashort central bond in bitetrahedrane, V. Galasso 181 (1994) 363

#### *Computational and simulation methods*

- Synergistic effects in bimolecular reactions in a dilute gas, A.S. Cukrowski, S. Fritzsche and W. Stiller 181 (1994) 7
- Equation of state of planar hard molecular fluids; hard cyclic multimer system, A.C. Brańka and K.W. Wojciechowski 181 (1994) 29
- A simple phenomenological model for nonequilibrium interaction between two reactions in a Lorentz gas, J. Gorecki and I. Hanazaki 181 (1994) 39
- A theoretical study of conformations and vibrational frequencies in  $(\text{NH}_2)_2\text{C}=\text{X}$  compounds ( $\text{X}=\text{O}, \text{S}, \text{and Se}$ ), T.-K. Ha and C. Puebla 181 (1994) 47
- Monte Carlo and molecular orbital study of the  $(\text{CH}_3)_2\text{NO}$  radical in solution, H. Takase and O. Kikuchi 181 (1994) 57
- Optical properties of linear mixed valence coordination compounds by two-band Hubbard Hamiltonian, A. Ferretti and A. Lami 181 (1994) 107
- Development of non-local Wigner-like correlation-energy density functionals through coordinate scaling requirements and evaluation of constraint obedience in the construction of density functionals, L.C. Wilson 181 (1994) 337
- Time-domain simulation of ESR spectra of nitroxide spin probes, H. Eviatar, E.E. van Faassen, Y.K. Levine and D.I. Hoult 181 (1994) 369

#### *Molecular dynamics and scattering theory*

- Optical, Raman and resonance Raman spectra and lattice dynamics calculations of the misfit layer compounds,  $(\text{SnS})_{1.17}\text{NbS}_2$  and  $(\text{PbS})_{1.18}\text{TiS}_2$ , C. Sourisseau, R. Cavagnat, M. Fouassier, J.L. Tirado and J. Morales 181 (1994) 377

#### **Experimental**

##### *Magnetic resonances*

- Time-resolved LMR measurement of the rate constants of the reactions  $\text{SiH}_3 + \text{SiH}_3$  and  $\text{SiH}_3 + \text{Cl}$ , A.V. Baklanov and A.I. Chichinin 181 (1994) 119
- Time-domain simulation of ESR spectra of nitroxide spin probes, H. Eviatar, E.E. van Faassen, Y.K. Levine and D.I. Hoult 181 (1994) 369

##### *Infrared spectroscopy*

- A matrix-isolation infrared spectroscopic study of the reactions of methane and methanol with ozone, C. Lugez, A. Schriver, R. Levant and L. Schriver-Mazzuoli 181 (1994) 129

- Vibrational dephasing of axial and equatorial conformers in cyclohexyl bromide, H. Abramczyk, M. Barut, A. Ben Altabef and R. Escibano 181 (1994) 393
- Vibrational dephasing of axial and equatorial conformers in cyclohexyl chloride and in 4-chloro-oxacyclohexane, A. Ben Altabef, R. Escibano and H. Abramczyk 181 (1994) 401
- Investigation of gas chemistry in the sealed TEA CO<sub>2</sub> laser, M.S. Trtica and Š.S. Miljanić 181 (1994) 409
- Raman spectroscopy*
- Optical, Raman and resonance Raman spectra and lattice dynamics calculations of the misfit layer compounds, (SnS)<sub>1.17</sub>NbS<sub>2</sub> and (PbS)<sub>1.18</sub>TiS<sub>2</sub>, C. Sourisseau, R. Cavagnat, M. Fouassier, J.L. Tirado and J. Morales 181 (1994) 377
- Vibrational dephasing of axial and equatorial conformers in cyclohexyl bromide, H. Abramczyk, M. Barut, A. Ben Altabef and R. Escibano 181 (1994) 393
- Vibrational dephasing of axial and equatorial conformers in cyclohexyl chloride and in 4-chloro-oxacyclohexane, A. Ben Altabef, R. Escibano and H. Abramczyk 181 (1994) 401
- Visible and UV spectroscopy*
- Valence- and inner-shell (Cl 2p, 2s; C 1s) photoabsorption and photoionization of carbon tetrachloride. Absolute oscillator strengths (5–400 eV) and dipole-induced breakdown pathways, G.R. Burton, W.F. Chan, G. Cooper and C.E. Brion 181 (1994) 147
- Double resonance spectroscopy of NaI and KI: the van der Waals states  $\Omega=1$  and  $\Omega=2$  of the first atomic asymptote, H. Bluhm, J. Lindner and E. Tiemann 181 (1994) 173
- High-resolution one- and two-photon spectra of matrix-isolated anthracene, J. Wolf and G. Hohlneicher 181 (1994) 185
- On the B state of the ICl molecule: hyperfine structure and hyperfine predissociation, A. Durand, J.C. Loison, G. Bazalgette, E. Gangler, F.W. Dalby and J. Vigué 181 (1994) 209
- Predissociation rates in carbon monoxide: dependence on rotational state, parity and isotope, K.S.E. Eikema, W. Hogervorst and W. Ubachs 181 (1994) 217
- Photoabsorption spectrum for OClO between 125 and 470 nm, S. Hubinger and J.B. Nee 181 (1994) 247
- Optical, Raman and resonance Raman spectra and lattice dynamics calculations of the misfit layer compounds, (SnS)<sub>1.17</sub>NbS<sub>2</sub> and (PbS)<sub>1.18</sub>TiS<sub>2</sub>, C. Sourisseau, R. Cavagnat, M. Fouassier, J.L. Tirado and J. Morales 181 (1994) 377
- Dual fluorescence of 9-anthryl-substituted oligothiophenes in nonpolar environment, P. Emele, D.U. Meyer, N. Holl, H. Port, H.C. Wolf, F. Würthner, P. Bäuerle and F. Effenberger 181 (1994) 417
- Fluorescence spectroscopy*
- The isomerization reaction of electronically excited (dibenzylmethine)borondifluoride in *n*-alcohols. Study of microscopic friction and polarity, T.O. Harju, J. Erostyák, Y.L. Chow and J.E.I. Korppi-Tommola 181 (1994) 259
- Fluorescence depolarization of solutions and ordered systems. Photochemical reactions in the excited states. II. General considerations (b), J.J. Fisz 181 (1994) 425
- Excited-state intramolecular proton transfer in jet-cooled 3-hydroxyflavone. Deuteration studies, vibronic double-resonance experiments, and semiempirical (AM1) calculations of potential-energy surfaces, A. Mühlpfordt, T. Bultmann, N.P. Ernsting and B. Dick 181 (1994) 447
- Photoelectron and Auger spectroscopy*
- Rydberg states of gas phase chlorobenzene observed by double resonance multiphoton ionization photoelectron spectroscopy, P. Asselin, F. Piuze, J. Le Calvé, M. Mons and I. Dimicoli 181 (1994) 271

- A He(I) photoelectron spectroscopic study of  $\text{MgF}_2$  in the gas phase, J.M. Dyke, D. Haggerston, M.P. Hastings and T.G. Wright 181 (1994) 355
- High-resolution Ge 3d and Sn 4d core-level photoelectron spectra. Ligand field and vibrational effects, J.N. Cutler, G.M. Bancroft and K.H. Tan 181 (1994) 461
- Electron impact spectroscopy*
- Valence- and inner-shell (Cl 2p, 2s; C 1s) photoabsorption and photoionization of carbon tetrachloride. Absolute oscillator strengths (5–400 eV) and dipole-induced breakdown pathways, G.R. Burton, W.F. Chan, G. Cooper and C.E. Brion 181 (1994) 147
- Laser methods*
- Time-resolved LMR measurement of the rate constants of the reactions  $\text{SiH}_3 + \text{SiH}_3$  and  $\text{SiH}_3 + \text{Cl}$ , A.V. Baklanov and A.I. Chichinin 181 (1994) 119
- Double resonance spectroscopy of NaI and KI: the van der Waals states  $\Omega=1$  and  $\Omega=2$  of the first atomic asymptote, H. Bluhm, J. Lindner and E. Tiemann 181 (1994) 173
- High-resolution one- and two-photon spectra of matrix-isolated anthracene, J. Wolf and G. Hohlneicher 181 (1994) 185
- Chain-length dependence of the quadratic hyperpolarizability of push–pull polyenes and carotenoids. Effect of end groups and conjugation path, M. Blanchard-Desce, J.-M. Lehn, M. Barzoukas, I. Ledoux and J. Zyss 181 (1994) 281
- Investigation of gas chemistry in the sealed TEA  $\text{CO}_2$  laser, M.S. Trtica and Š.S. Miljanić 181 (1994) 409
- Picosecond spectroscopy*
- The isomerization reaction of electronically excited (dibenzylmethine)borondifluoride in *n*-alcohols. Study of microscopic friction and polarity, T.O. Harju, J. Erostryák, Y.L. Chow and J.E.I. Korppi-Tommola 181 (1994) 259
- Dual fluorescence of 9-anthryl-substituted oligothiophenes in nonpolar environment, P. Emele, D.U. Meyer, N. Holl, H. Port, H.C. Wolf, F. Würthner, P. Bäuerle and F. Effenberger 181 (1994) 417
- Fluorescence depolarization of solutions and ordered systems. Photochemical reactions in the excited states. II. General considerations (b), J.J. Fisz 181 (1994) 425
- Non-linear optical spectroscopy*
- Chain-length dependence of the quadratic hyperpolarizability of push–pull polyenes and carotenoids. Effect of end groups and conjugation path, M. Blanchard-Desce, J.-M. Lehn, M. Barzoukas, I. Ledoux and J. Zyss 181 (1994) 281
- Multiple resonance spectroscopy*
- Rydberg states of gas phase chlorobenzene observed by double resonance multiphoton ionization photoelectron spectroscopy, P. Asselin, F. Piuze, J. Le Calvé, M. Mons and I. Dimicoli 181 (1994) 271
- Time-resolved experiments*
- Time-resolved LMR measurement of the rate constants of the reactions  $\text{SiH}_3 + \text{SiH}_3$  and  $\text{SiH}_3 + \text{Cl}$ , A.V. Baklanov and A.I. Chichinin 181 (1994) 119

## Objects

### Bulk systems

#### Gases

- Synergistic effects in bimolecular reactions in a dilute gas, A.S. Cukrowski, S. Fritzsche and W. Stiller 181 (1994) 7
- A simple phenomenological model for nonequilibrium interaction between two reactions in a Lorentz gas, J. Gorecki and I. Hanazaki 181 (1994) 39
- A new drift-velocity formula for ions in lighter gases in an electric field, L. Ferrari 181 (1994) 319
- High-resolution Ge 3d and Sn 4d core-level photoelectron spectra. Ligand field and vibrational effects, J.N. Cutler, G.M. Bancroft and K.H. Tan 181 (1994) 461

#### Liquids mixtures and solutions

- Monte Carlo and molecular orbital study of the  $(\text{CH}_3)_2\text{NO}$  radical in solution, H. Takase and O. Kikuchi 181 (1994) 57
- The isomerization reaction of electronically excited (dibenzylmethine)borondifluoride in *n*-alcohols. Study of microscopic friction and polarity, T.O. Harju, J. Erostryák, Y.L. Chow and J.E.I. Korppi-Tommola 181 (1994) 259
- Chain-length dependence of the quadratic hyperpolarizability of push-pull polyenes and carotenoids. Effect of end groups and conjugation path, M. Blanchard-Desce, J.-M. Lehn, M. Barzoukas, I. Ledoux and J. Zyss 181 (1994) 281
- Vibrational dephasing of axial and equatorial conformers in cyclohexyl chloride and in 4-chloro-oxacyclohexane, A. Ben Altabef, R. Escribano and H. Abramczyk 181 (1994) 401
- Fluorescence depolarization of solutions and ordered systems. Photochemical reactions in the excited states. II. General considerations (b), J.J. Fisz 181 (1994) 425

#### Glasses

- On the interpretation of the external heavy atom effect on singlet-triplet transitions, B.F. Minaev, S. Knuts and H. Ågren 181 (1994) 15

#### Liquid crystals

- Time-domain simulation of ESR spectra of nitroxide spin probes, H. Eviatar, E.E. van Faassen, Y.K. Levine and D.I. Hoult 181 (1994) 369
- Fluorescence depolarization of solutions and ordered systems. Photochemical reactions in the excited states. II. General considerations (b), J.J. Fisz 181 (1994) 425

#### Metals and alloys

- Optical, Raman and resonance Raman spectra and lattice dynamics calculations of the misfit layer compounds,  $(\text{SnS})_{1.17}\text{NbS}_2$  and  $(\text{PbS})_{1.18}\text{TiS}_2$ , C. Sourisseau, R. Cavagnat, M. Fouassier, J.L. Tirado and J. Morales 181 (1994) 377

#### Surfaces

- Chemisorption of aluminium and chlorine on the Si(111) surface. An ab initio study of the nature of the interaction, C. Bo, J.M. Maestre, J.M. Poblet and J.M. Ricart 181 (1994) 63

*Low-dimensional materials*

- Equation of state of planar hard molecular fluids; hard cyclic multimer system, A.C. Brańka and K.W. Wojciechowski 181 (1994) 29
- Optical properties of linear mixed valence coordination compounds by two-band Hubbard Hamiltonian, A. Ferretti and A. Lami 181 (1994) 107
- Optical, Raman and resonance Raman spectra and lattice dynamics calculations of the misfit layer compounds,  $(\text{SnS})_{1.17}\text{NbS}_2$  and  $(\text{PbS})_{1.18}\text{TiS}_2$ , C. Sourisseau, R. Cavagnat, M. Fouassier, J.L. Tirado and J. Morales 181 (1994) 377

*Plasmas*

- Investigation of gas chemistry in the sealed TEA  $\text{CO}_2$  laser, M.S. Trtica and Š.S. Miljanić 181 (1994) 409

**Microscopic systems***Atoms*

- Development of non-local Wigner-like correlation-energy density functionals through coordinate scaling requirements and evaluation of constraint obedience in the construction of density functionals, L.C. Wilson 181 (1994) 337

*Molecules (neutral and ionic)*

- Synergistic effects in bimolecular reactions in a dilute gas, A.S. Cukrowski, S. Fritzsche and W. Stiller 181 (1994) 7
- A theoretical study of conformations and vibrational frequencies in  $(\text{NH}_2)_2\text{C}=\text{X}$  compounds ( $\text{X}=\text{O}$ , S, and Se), T.-K. Ha and C. Puebla 181 (1994) 47
- Dissociation dynamics of acetyl chloride and cis-trans isomerisation of methoxychloro carbene and chlorohydroxymethyl carbene, R. Sumathi and A.K. Chandra 181 (1994) 73
- LCAO expansion in a spline basis for accurate variational determination of continuum wavefunctions. Applications to  $\text{H}_2^+$  and  $\text{HeH}^{2+}$ , M. Brosolo, P. Decleva and A. Lisini 181 (1994) 85
- Radiative lifetimes of triplet spin sublevels of the azabenzenes, H. Ågren, O. Vahtras, S. Knuts and P. Jørgensen 181 (1994) 291
- Investigation of gas chemistry in the sealed TEA  $\text{CO}_2$  laser, M.S. Trtica and Š.S. Miljanić 181 (1994) 409
- Dual fluorescence of 9-anthryl-substituted oligothiophenes in nonpolar environment, P. Emele, D.U. Meyer, N. Holl, H. Port, H.C. Wolf, F. Würthner, P. Bäuerle and F. Effenberger 181 (1994) 417

*-diatomic*

- Double resonance spectroscopy of NaI and KI: the van der Waals states  $\Omega=1$  and  $\Omega=2$  of the first atomic asymptote, H. Bluhm, J. Lindner and E. Tiemann 181 (1994) 173
- On the B state of the ICl molecule: hyperfine structure and hyperfine predissociation, A. Durand, J.C. Loison, G. Bazalgette, E. Gangler, F.W. Dalby and J. Vigué 181 (1994) 209
- Predissociation rates in carbon monoxide: dependence on rotational state, parity and isotope, K.S.E. Eikema, W. Hogervorst and W. Ubachs 181 (1994) 217

*-small polyatomics*

- On the interpretation of the external heavy atom effect on singlet-triplet transitions, B.F. Minaev, S. Knuts and H. Ågren 181 (1994) 15
- Chemisorption of aluminium and chlorine on the Si(111) surface. An ab initio study of the nature of the interaction, C. Bo, J.M. Maestre, J.M. Poblet and J.M. Ricart 181 (1994) 63

- Dissociation dynamics of acetyl chloride and *cis-trans* isomerisation of methoxychloro carbene and chlorohydroxymethyl carbene, R. Sumathi and A.K. Chandra 181 (1994) 73
- Energy-component analysis along zero virial path, H. Tokiwa, Y. Osamura and H. Ichikawa 181 (1994) 97
- Valence- and inner-shell (Cl 2p, 2s; C 1s) photoabsorption and photoionization of carbon tetrachloride. Absolute oscillator strengths (5–400 eV) and dipole-induced breakdown pathways, G.R. Burton, W.F. Chan, G. Cooper and C.E. Brion 181 (1994) 147
- Photoabsorption spectrum for OClO between 125 and 470 nm, S. Hubinger and J.B. Nee 181 (1994) 247
- A He(I) photoelectron spectroscopic study of MgF<sub>2</sub> in the gas phase, J.M. Dyke, D. Haggerston, M.P. Hastings and T.G. Wright 181 (1994) 355
- High-resolution Ge 3d and Sn 4d core-level photoelectron spectra. Ligand field and vibrational effects, J.N. Cutler, G.M. Bancroft and K.H. Tan 181 (1994) 461
- aromatics*
- High-resolution one- and two-photon spectra of matrix-isolated anthracene, J. Wolf and G. Hohlneicher 181 (1994) 185
- Rydberg states of gas phase chlorobenzene observed by double resonance multiphoton ionization photoelectron spectroscopy, P. Asselin, F. Piuze, J. Le Calvé, M. Mons and I. Dimicoli 181 (1994) 271
- Excited-state intramolecular proton transfer in jet-cooled 3-hydroxyflavone. Deuteration studies, vibronic double-resonance experiments, and semiempirical (AM1) calculations of potential-energy surfaces, A. Mühlfordt, T. Bultmann, N.P. Ernsting and B. Dick 181 (1994) 447
- other large*
- Chain-length dependence of the quadratic hyperpolarizability of push-pull polyenes and carotenoids. Effect of end groups and conjugation path, M. Blanchard-Desce, J.-M. Lehn, M. Barzoukas, I. Ledoux and J. Zyss 181 (1994) 281
- Molecular aggregates*
- dimers*
- Isotope effects in weak hydrogen bonds. Allowance for two stretching and two bending modes of the A–H...B fragment, N.D. Sokolov and V.A. Savel'ev 181 (1994) 305
- van der Waals molecules*
- Isotope effects in weak hydrogen bonds. Allowance for two stretching and two bending modes of the A–H...B fragment, N.D. Sokolov and V.A. Savel'ev 181 (1994) 305
- clusters*
- Vibronic reduction of electron transfer in strongly correlated molecular models, S.A. Borshch and J.-J. Girerd 181 (1994) 1
- complexes*
- On the interpretation of the external heavy atom effect on singlet-triplet transitions, B.F. Minaev, S. Knuts and H. Ågren 181 (1994) 15
- Optical properties of linear mixed valence coordination compounds by two-band Hubbard Hamiltonian, A. Ferretti and A. Lami 181 (1994) 107
- A matrix-isolation infrared spectroscopic study of the reactions of methane and methanol with ozone, C. Lugez, A. Schriver, R. Levant and L. Schriver-Mazzuoli 181 (1994) 129

*Free radicals (including hydronium and muonium)*

- Monte Carlo and molecular orbital study of the  $(\text{CH}_3)_2\text{NO}$  radical in solution, H. Takase and O. Kikuchi 181 (1994) 57
- Time-resolved LMR measurement of the rate constants of the reactions  $\text{SiH}_3 + \text{SiH}_3$  and  $\text{SiH}_3 + \text{Cl}$ , A.V. Baklanov and A.I. Chichinin 181 (1994) 119

*Ions and charge carriers*

- A new drift-velocity formula for ions in lighter gases in an electric field, L. Ferrari 181 (1994) 319
- Development of non-local Wigner-like correlation-energy density functionals through coordinate scaling requirements and evaluation of constraint obedience in the construction of density functionals, L.C. Wilson 181 (1994) 337

**Phenomena***Molecular structure*

- A theoretical study of conformations and vibrational frequencies in  $(\text{NH}_2)_2\text{C}=\text{X}$  compounds ( $\text{X}=\text{O}$ , S, and Se), T.-K. Ha and C. Puebla 181 (1994) 47
- Chemisorption of aluminium and chlorine on the  $\text{Si}(111)$  surface. An ab initio study of the nature of the interaction, C. Bo, J.M. Maestre, J.M. Poblet and J.M. Ricart 181 (1994) 63
- Theoretical study of the nuclear spin-spin coupling constant of the ultrashort central bond in bitetrahedrane, V. Galasso 181 (1994) 363
- Vibrational dephasing of axial and equatorial conformers in cyclohexyl bromide, H. Abramczyk, M. Barut, A. Ben Altabef and R. Escibano 181 (1994) 393
- Excited-state intramolecular proton transfer in jet-cooled 3-hydroxyflavone. Deuteration studies, vibronic double-resonance experiments, and semiempirical (AM1) calculations of potential-energy surfaces, A. Mühlfordt, T. Bultmann, N.P. Ernsting and B. Dick 181 (1994) 447

*Vibrations and rotations of molecules*

- A theoretical study of conformations and vibrational frequencies in  $(\text{NH}_2)_2\text{C}=\text{X}$  compounds ( $\text{X}=\text{O}$ , S, and Se), T.-K. Ha and C. Puebla 181 (1994) 47
- Rydberg states of gas phase chlorobenzene observed by double resonance multiphoton ionization photoelectron spectroscopy, P. Asselin, F. Piuze, J. Le Calvé, M. Mons and I. Dimicoli 181 (1994) 271
- Vibrational dephasing of axial and equatorial conformers in cyclohexyl bromide, H. Abramczyk, M. Barut, A. Ben Altabef and R. Escibano 181 (1994) 393
- Vibrational dephasing of axial and equatorial conformers in cyclohexyl chloride and in 4-chloro-oxacyclohexane, A. Ben Altabef, R. Escibano and H. Abramczyk 181 (1994) 401

*Electronic structure and states*

- On the interpretation of the external heavy atom effect on singlet-triplet transitions, B.F. Minaev, S. Knuts and H. Ågren 181 (1994) 15
- Monte Carlo and molecular orbital study of the  $(\text{CH}_3)_2\text{NO}$  radical in solution, H. Takase and O. Kikuchi 181 (1994) 57
- Dissociation dynamics of acetyl chloride and cis-trans isomerisation of methoxychloro carbene and chlorohydroxymethyl carbene, R. Sumathi and A.K. Chandra 181 (1994) 73

- LCAO expansion in a spline basis for accurate variational determination of continuum wavefunctions. Applications to  $H_2^+$  and  $HeH^{2+}$ , M. Brosolo, P. Decleva and A. Lisini 181 (1994) 85
- Double resonance spectroscopy of NaI and KI: the van der Waals states  $\Omega=1$  and  $\Omega=2$  of the first atomic asymptote, H. Bluhm, J. Lindner and E. Tiemann 181 (1994) 173
- High-resolution one- and two-photon spectra of matrix-isolated anthracene, J. Wolf and G. Hohlneicher 181 (1994) 185
- Photoabsorption spectrum for OCIO between 125 and 470 nm, S. Hubinger and J.B. Nee 181 (1994) 247
- Rydberg states of gas phase chlorobenzene observed by double resonance multiphoton ionization photoelectron spectroscopy, P. Asselin, F. Piuze, J. Le Calvé, M. Mons and I. Dimicoli 181 (1994) 271
- A He(I) photoelectron spectroscopic study of  $MgF_2$  in the gas phase, J.M. Dyke, D. Haggerston, M.P. Hastings and T.G. Wright 181 (1994) 355
- Electric and magnetic properties*
- Optical properties of linear mixed valence coordination compounds by two-band Hubbard Hamiltonian, A. Ferretti and A. Lami 181 (1994) 107
- A new drift-velocity formula for ions in lighter gases in an electric field, L. Ferrari 181 (1994) 319
- Spin splittings*
- On the B state of the ICl molecule: hyperfine structure and hyperfine predissociation, A. Durand, J.C. Loison, G. Bazalgette, E. Gangler, F.W. Dalby and J. Vigué 181 (1994) 209
- Molecular interactions*
- Isotope effects in weak hydrogen bonds. Allowance for two stretching and two bending modes of the A-H...B fragment, N.D. Sokolov and V.A. Savel'ev 181 (1994) 305
- Vibrational dephasing of axial and equatorial conformers in cyclohexyl bromide, H. Abramczyk, M. Barut, A. Ben Altabef and R. Escibano 181 (1994) 393
- Vibrational dephasing of axial and equatorial conformers in cyclohexyl chloride and in 4-chloro-oxacyclohexane, A. Ben Altabef, R. Escibano and H. Abramczyk 181 (1994) 401
- Fluorescence depolarization of solutions and ordered systems. Photochemical reactions in the excited states. II. General considerations (b), J.J. Fisz 181 (1994) 425
- Spectral bandshapes and intensities*
- Optical properties of linear mixed valence coordination compounds by two-band Hubbard Hamiltonian, A. Ferretti and A. Lami 181 (1994) 107
- Valence- and inner-shell (Cl 2p, 2s; C 1s) photoabsorption and photoionization of carbon tetrachloride. Absolute oscillator strengths (5–400 eV) and dipole-induced breakdown pathways, G.R. Burton, W.F. Chan, G. Cooper and C.E. Brion 181 (1994) 147
- Coupling of electronic and nuclear motion*
- Vibronic reduction of electron transfer in strongly correlated molecular models, S.A. Borshch and J.-J. Girerd 181 (1994) 1
- On the B state of the ICl molecule: hyperfine structure and hyperfine predissociation, A. Durand, J.C. Loison, G. Bazalgette, E. Gangler, F.W. Dalby and J. Vigué 181 (1994) 209
- Molecular photophysical processes*
- A matrix-isolation infrared spectroscopic study of the reactions of methane and methanol with ozone, C. Lugez, A. Schriver, R. Levant and L. Schriver-Mazzuoli 181 (1994) 129

- Predissociation rates in carbon monoxide: dependence on rotational state, parity and isotope, K.S.E. Eikema, W. Hogervorst and W. Ubachs 181 (1994) 217
- Photoabsorption spectrum for OClO between 125 and 470 nm, S. Hubinger and J.B. Nee 181 (1994) 247
- Dual fluorescence of 9-anthryl-substituted oligothiophenes in nonpolar environment, P. Emele, D.U. Meyer, N. Holl, H. Port, H.C. Wolf, F. Würthner, P. Bäuerle and F. Effenberger 181 (1994) 417
- High-resolution Ge 3d and Sn 4d core-level photoelectron spectra. Ligand field and vibrational effects, J.N. Cutler, G.M. Bancroft and K.H. Tan 181 (1994) 461
- Intramolecular dynamics*
- Excited-state intramolecular proton transfer in jet-cooled 3-hydroxyflavone. Deuteration studies, vibronic double-resonance experiments, and semiempirical (AM1) calculations of potential-energy surfaces, A. Mühlpfordt, T. Bultmann, N.P. Ernsting and B. Dick 181 (1994) 447
- radiationless transitions*
- On the B state of the ICl molecule: hyperfine structure and hyperfine predissociation, A. Durand, J.C. Loison, G. Bazalgette, E. Gangler, F.W. Dalby and J. Vigué 181 (1994) 209
- The isomerization reaction of electronically excited (dibenzylmethine)borondifluoride in *n*-alcohols. Study of microscopic friction and polarity, T.O. Harju, J. Eroestyák, Y.L. Chow and J.E.I. Korppi-Tommola 181 (1994) 259
- Luminescence spectra, yields and lifetimes*
- Dual fluorescence of 9-anthryl-substituted oligothiophenes in nonpolar environment, P. Emele, D.U. Meyer, N. Holl, H. Port, H.C. Wolf, F. Würthner, P. Bäuerle and F. Effenberger 181 (1994) 417
- Non-linear responses (including optical)*
- Chain-length dependence of the quadratic hyperpolarizability of push-pull polyenes and carotenoids. Effect of end groups and conjugation path, M. Blanchard-Desce, J.-M. Lehn, M. Barzoukas, I. Ledoux and J. Zyss 181 (1994) 281
- Multiphoton phenomena*
- High-resolution one- and two-photon spectra of matrix-isolated anthracene, J. Wolf and G. Hohlneicher 181 (1994) 185
- Theoretical study of the nuclear spin-spin coupling constant of the ultrashort central bond in bitetrahedrane, V. Galasso 181 (1994) 363
- Reactions (including dissociation)*
- A simple phenomenological model for nonequilibrium interaction between two reactions in a Lorentz gas, J. Gorecki and I. Hanazaki 181 (1994) 39
- gas phase*
- Synergistic effects in bimolecular reactions in a dilute gas, A.S. Cukrowski, S. Fritzsche and W. Stiller 181 (1994) 7
- Time-resolved LMR measurement of the rate constants of the reactions  $\text{SiH}_3 + \text{SiH}_3$  and  $\text{SiH}_3 + \text{Cl}$ , A.V. Baklanov and A.I. Chichinin 181 (1994) 119
- Investigation of gas chemistry in the sealed TEA  $\text{CO}_2$  laser, M.S. Trtica and Š.S. Miljanić 181 (1994) 409

*Electron transfer*

- Vibronic reduction of electron transfer in strongly correlated molecular models, S.A. Borshch and J.-J. Girerd 181 (1994) 1

*Ionization (including Rydberg states)*

- LCAO expansion in a spline basis for accurate variational determination of continuum wavefunctions. Applications to  $H_2^+$  and  $HeH^{2+}$ , M. Brosolo, P. Decleva and A. Lisini 181 (1994) 85
- Valence- and inner-shell (Cl 2p, 2s; C 1s) photoabsorption and photoionization of carbon tetrachloride. Absolute oscillator strengths (5–400 eV) and dipole-induced breakdown pathways, G.R. Burton, W.F. Chan, G. Cooper and C.E. Brion 181 (1994) 147
- A He(I) photoelectron spectroscopic study of  $MgF_2$  in the gas phase, J.M. Dyke, D. Haggerston, M.P. Hastings and T.G. Wright 181 (1994) 355

*Molecular motion (including diffusive)*

- The isomerization reaction of electronically excited (dibenzylmethine)borondifluoride in *n*-alcohols. Study of microscopic friction and polarity, T.O. Harju, J. Erostryák, Y.L. Chow and J.E.I. Korppi-Tommola 181 (1994) 259
- Time-domain simulation of ESR spectra of nitroxide spin probes, H. Eviatar, E.E. van Faassen, Y.K. Levine and D.I. Hoult 181 (1994) 369

*Isotopic effects*

- Isotope effects in weak hydrogen bonds. Allowance for two stretching and two bending modes of the A–H...B fragment, N.D. Sokolov and V.A. Savel'ev 181 (1994) 305

*Surface effects and catalysis*

- Chemisorption of aluminium and chlorine on the Si(111) surface. An ab initio study of the nature of the interaction, C. Bo, J.M. Maestre, J.M. Poblet and J.M. Ricart 181 (1994) 63

*Thermodynamic and transport properties*

- Equation of state of planar hard molecular fluids; hard cyclic multimer system, A.C. Brańka and K.W. Wojciechowski 181 (1994) 29
- A new drift-velocity formula for ions in lighter gases in an electric field, L. Ferrari 181 (1994) 319

